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Proximity effect in atomic-scaled hybrid superconductor/ferromagnet structures: crucial role of electron spectra.

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Abstract. - We study the influence of the configuration of the majority and minority spin subbands of electron spectra on the properties of atomic-scaled superconductor-ferromagnet S-F-S and F-S-F hybrid structures. At low temperatures, the S/F/S junction is either a 0 or junction depending on the energy shift between S and F materials and the anisotropy of the Fermi surfaces. We found that the spin switch effect in F/S/F system can be reversed if the minority spin electron spectra in F metal is of the hole-like type.

1. Introduction- Phenomena arising in the superconductor-ferromagnet (S/F) heterostructures attract a growing interest due to their potential application in spintronic and quantum computation devices [1-3]. For example, the so-called spin-switch effect (SSE) (also called spin-valve effect) occurs when the critical temperature of the superconductor in the F/S/F structure depends on the mutual orientation of the ferromagnetic layers magnetizations. Moreover the S/F/S $\pi-$junctions with the changing superconducting order parameter phase shift are good candidates for the quantum computer elements, q-bit [4].

Critical current oscillations as a function of the exchange field and thickness of the ferromagnetic spacer in a S/F/S Josephson junctions have been predicted [5] and associated with the $0-\pi$ phase transition. Experimentally the evidence of such $0-\pi$ phase transition has been obtained first for the nanoscaled Josephson junctions S/F/S with a weak ferromagnetic interlayers in Cu_xNi_{1-x} [6] and PdNi alloys [7]. The $0-\pi$ phase transition was also predicted in layered compounds within a simple model of alternating F and S atomic layers [8-9]. This prediction is relevant for ruthenocuprates $RuSr_2GdCu_2O_8$ which are natural S/F layered compounds [10].

The F/S/F trilayer also exhibits interesting spin dependent phenomena. It was predicted [11-13] and observed [14-19] that the critical temperature is higher for antiparallel (AP) magnetization configuration than for the parallel (P) one. Besides this so called normal SSE, several recent experiments report on an inverse SSE whereby the parallel configuration is more favorable for the superconductivity than the antiparallel one [20-25].

The situation with inverse SSE investigated in [20] is somewhere controversial because in the similar Py/Nb/Py system in [21] the normal SSE was observed. The possible explanation of the inverse SSE observed in [20] has been recentlty proposed in [26] and it is related with a
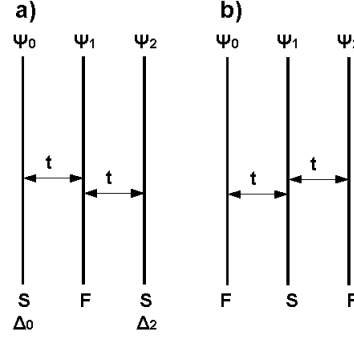
Fig. 1: Geometry of the three-layer system. Here ψ_0, ψ_1 and ψ_2 are the electron annihilation operators in the corresponding layer.

stray magnetic field generated in the AP configuration. The similar arguments may explain inverse SSE observed in [22,23]. However this reasoning do not work for the inverse SSE revealed in [24] where the magnetizations were perpendicular to the layers. therefoe due to the demagnetization the influence of orbital effect was excluded.

In this letter, we investigate the $0 - \pi$ phase transition and SSE for more realistic band structure. In particular, the $\pi-$phase might be suppressed when the ferromagnet bands are sufficiently energy-shifted with respect to the superconductor ones. The anisotropy of the quasi particle spectra is also of primary importance for the $0 - \pi$ phase transition. This could explain why the $\pi-$phase was not observed in Ruthenocuprates [27]. Furthermore, if the majority and minority spin subbands have opposite electron/hole character, we predict the inverse SSE providing a possible explanation of results [24].

2. Model - We start with an exactly solvable model [8] of alternating superconducting and ferromagnetic atomic metallic layers. The electron's motion is described in the F layers by the spin-dependent energy spectrum $\xi_\sigma(\mathbf{k})$ and by spin independent energy spectrum $\xi_s(\mathbf{k})$ in the S layers. Three basic parameters characterize the system : t is the transfer energy between the F and S layers, λ is the Cooper pairing constant which is assumed to be nonzero in S layers only, and h is the constant exchange field in the F layers only. It is supposed that the coupling between the layers is realized via the transfer integral t, which is relatively small ($t \ll T_c$), so the superconductivity can coexist with ferromagnetism in the adjacent layers. The Hamiltonian of the system can be written as $H = H_0 + H_{BCS} + H_t$ with:

$$H_0 = \sum_{n,\sigma,\mathbf{k}} \left[\xi_\sigma^n(\mathbf{k}) \psi_{\sigma,n}^+(\mathbf{k}) \psi_{\sigma,n}(\mathbf{k}) \right], \tag{1}$$

$$H_{BCS} = \sum_{n,\mathbf{k}} \left[\Delta_n^* \psi_{\downarrow,n}^+(\mathbf{k}) \psi_{\uparrow,n}^+(-\mathbf{k}) + \Delta_n \psi_{\uparrow,n}(\mathbf{k}) \psi_{\downarrow,n}(-\mathbf{k}) \right], \tag{2}$$

$$H_t = t \sum_{n,\sigma,\mathbf{k}} \left[\psi_{\sigma,(n+1)}^+(\mathbf{k}) \psi_{\sigma,n}(\mathbf{k}) + \psi_{\sigma,n}^+(\mathbf{k}) \psi_{\sigma,(n+1)}(\mathbf{k}) \right], \tag{3}$$

where $\psi_{\sigma,n}^+(\mathbf{k})$ is the creation operator of an electron with spin σ and momentum $\mathbf{k}$ in the nth layer. The BCS pairing in the S layers is treated in H_{BCS} in a mean-field approximation [28]. The superconducting order parameter Δ_n is non zero only in the S layers. Note that the electrons spectra in (3) are calculated from the Fermi energy. As usual, we introduce the normal and anomalous Green functions [28] $G_{\sigma,\sigma'}^{n,m} = - \left\langle T_\tau \left(\psi_{\sigma,n}(\mathbf{k}) \psi_{\sigma',m}^+(\mathbf{k}) \right) \right\rangle$ and

$\widetilde{F}_{\sigma,\sigma'}^{n,m} = \left\langle T_\tau \left(\psi_{\sigma,n}^+ (\mathbf{k}) \psi_{\sigma',m}^+ (-\mathbf{k}) \right) \right\rangle$ which satisfy the system of equations:

$$(i\omega - \xi_\sigma^n) G_{\sigma,\sigma'}^{n,m} - tG_{\sigma,\sigma'}^{n-1,m} - tG_{\sigma,\sigma'}^{n+1,m} + \Delta_n^* \widetilde{F}_{-\sigma,\sigma'}^{n,m} = \delta_{nm},$$
$$(i\omega + \xi_{-\sigma}^n) \widetilde{F}_{-\sigma,\sigma'}^{n,m} + t\widetilde{F}_{-\sigma,\sigma'}^{n-1,m} + t\widetilde{F}_{\sigma,\sigma'}^{n+1,m} + \Delta_n G_{\sigma,\sigma'}^{n,m} = 0, \tag{4}$$

where $\omega = (2l+1)\pi T_c$ are the fermion Matsubara's frequencies, $\xi_\sigma^n = \xi_\sigma^n (\mathbf{k})$ and n and m the layers indices. The superconducting order parameter in the nth layer satisfies the standard self-consistency equation

$$\Delta_n^* = |\lambda| T \sum_\omega \sum_{\mathbf{k}} \widetilde{F}_{-\sigma,\sigma'}^{n,m}. \tag{5}$$

The anomalous Green function $\widetilde{F}_{-\sigma,\sigma'}^{n,m}$ of the system (5) can be be expressed by means of normal Green functions

$$\widetilde{F}_{-\sigma,\sigma'}^{n,m} = \sum_p \Delta_{n-l}^* G_{-\sigma,\sigma'}^{\omega;n-p,m} G_{0,\sigma,-\sigma'}^{-\omega;p,m},$$

where G_0 is the Green function in the absence of superconductivity pairing, i.e. for $\Delta_n = 0$.

3. $0-\pi$ phase transition in S/F/S system - In this section we examine the phase difference between the order parameters in the adjacent superconducting layers of the S/F/S system (see figure 1 (a)). Here $n = 0,2$ and $\xi_{s,0} = \xi_{s,2} = \xi_s$ for the S layers, and $n = 1$ with $\xi_{\sigma,1} = \xi_\sigma$ for the F layer. Due to the symmetry reason the order parameters of both S layers may differ from each other in the phase prefactor $e^{i\varphi}$ and $|\Delta_0| = |\Delta_2|$ (in fact only the situation with $\Delta_0 = \pm\Delta_2$ is possible).

Solving the system of equation (4) in the case of the trilayer , we find the anomalous Green functions of the S layers. Using them, the self-consistency equation (5) can be written as :

$$\Delta_0^* = -\lambda T \left\{ \sum_{\omega,\mathbf{k}} \left[G_{\uparrow\uparrow}^{\omega;0,0} \Delta_0^* G_{0\downarrow\downarrow}^{-\omega;0,0} + G_{\uparrow\uparrow}^{\omega;2,0} \Delta_2^* G_{0\downarrow\downarrow}^{-\omega;2,0} \right] \right\}. \tag{6}$$

where

$$G_{0\uparrow\uparrow}^{0,0} = \frac{\left(a_\uparrow^* - t^2\right)}{(i\omega - \xi_s)\left[\left(a_\uparrow^* - 2t^2\right)\right]}, G_{0,\uparrow\uparrow}^{2,0} = \frac{t^2}{(i\omega - \xi_s)\left[\left(a_\uparrow^* - 2t^2\right)\right]},$$

with $a_\sigma = (i\omega + \xi_\sigma)(i\omega + \xi_s)$. The transition between 0 and π states implies a change of the relative sign between Δ_0 and Δ_2. Near T_c, taking into account that in $0-$phase, $\Delta_0 = +\Delta_2$ and in the $\pi-$phase, $\Delta_0 = -\Delta_2$, the combination of the self consistency equations (6) written in $0-$phase and $\pi-$phase provides one with the following expression

$$\ln \left(\frac{T_c^0}{T_c^\pi} \right) = 2T_{c0} \sum_{\omega,\mathbf{k}} G_{0\uparrow\uparrow}^{\omega;2,0} G_{0\downarrow\downarrow}^{-\omega;2,0}, \tag{7}$$

where T_c^0 is the superconducting critical temperature when the system is in the $0-$phase, T_c^π is the superconducting critical temperature when the system is in the $\pi-$phase and T_{c0} is the bare mean-field critical temperature of the single superconductivity layer. The logarithm can be simplified as $\ln \left(T_c^0 / T_c^\pi \right) \simeq \left(T_c^0 - T_c^\pi \right) / T_c^0 = \Delta T / T_c^0$ because the critical temperature variation is small $\left(\left(T_c^0 - T_c^\pi \right) / T_c^0 \ll 1 \right)$.

The sign of the right hand side in (7) determines whether it is 0 or $\pi-$phase which is realized. Indeed, the transition occurs in the state with higher critical temperature. We are interested in the situation when the right hand side in (7) is negative, i.e. $T_c^\pi > T_c^0$ and we deal with the $\pi-$phase difference of order parameters between the two superconducting layers.

First, we concentrate on the case with isotropic electron's dispersion when Fermi surfaces are circular. The calculation of the critical temperature, in the case of isotropic Fermi surface and symmetrical ferromagnet energy band splitting $\xi^{\uparrow(\downarrow)} = \xi_s \mp h$ has been performed in [9]. Here we address the more general case with $\xi_\uparrow = \xi_s + E^\uparrow$ and $\xi_\downarrow = \xi_s + E^\downarrow$ where $E^{\uparrow(\downarrow)}$ is the energy difference of the electron energy spectrum with spin up (down) compared to the superconductor energy spectrum ξ_s. The calculation of the sum over momentum $\mathbf{k}$ in (7) may be transformed into an integration over ξ_s, i.e. $\sum_k \longrightarrow N(0) \int \int d\xi_s d\theta$, where $N(0)$ is the density of state at the Fermi energy E_F. Performing the integration over energy ξ_s we confronted with several possible situations according to the values and signs of $E^\uparrow$ and $E^\downarrow$ that may be classified as follows : 1) $E^\uparrow \gg T_{c0}$, but $E^\downarrow$ is of the order of T_{c0}, 2) $E^\uparrow \gg T_{c0}$, $E^\downarrow \gg T_{c0}$ and 3) $E^\uparrow \gg T_{c0}$, $E^\downarrow \ll T_{c0}$.

In the case 1) when $E^\uparrow \gg T_{c0}$ and $E^\downarrow$ is of the order of T_{c0}, the electrons up energy band is strongly shifted in comparison to the superconductor one and electrons down have energy band close to the superconductor one. The critical temperature difference in the limit $t \ll T_c$,with $\omega > 0$, becomes :

$$\frac{\Delta T}{T_c^0} = \frac{7\pi t^4 \zeta(3)}{8E^\uparrow E^\downarrow \pi^3 T_{c0}^2} - \frac{t^4}{8E^\uparrow E^{\downarrow 2}\pi T_{c0}} \operatorname{Im}\left(\Psi'\left(\frac{1}{2} - \frac{iE^\downarrow}{4\pi T_{c0}}\right)\right). \tag{8}$$

where Ψ' is the first derivative digamma function. From (8) we deduce that $\Delta T = T_c^0 - T_c^\pi > 0$ and the S/F/S system is in the $0-$phase if $E^\uparrow$ and $E^\downarrow$ have both the same sign. However, $\Delta T < 0$ and the S/F/S system is in the $\pi-$phase if $E^\uparrow$ and $E^\downarrow$ have opposite sign $e.g.$ $E^\uparrow$ positive and $E^\downarrow$ negative. Thus, the existence of the $\pi-$phase depends on the energy band shift between the ferromagnetic spectra and the superconductors spectra.

If we switch the role of $E^\downarrow$ and $E^\uparrow$ in (7) i.e. $E^\downarrow \gg T_{c0}$ and $E^\uparrow$ is of the order of T_{c0}, the conclusions are similar. When $E^\uparrow$ and $E^\downarrow$ have both the same sign, the S/F/S system is in the $0-$phase. When $E^\uparrow$ and $E^\downarrow$ have opposite sign, the S/F/S system is in the $\pi-$phase.

In the case 2), when $E^\uparrow \gg T_{c0}$ and $E^\downarrow \gg T_{c0}$, the electrons up and down have both a strong energy band shift compared to the superconducting energy spectrum. The critical temperature difference becomes $\Delta T/T_c^0 = 7\pi t^4 \zeta(3)/(8E^\uparrow E^\downarrow \pi^3 T_{c0}^2)$. The $\pi-$phase only appears if $E^\uparrow$ and $E^\downarrow$ have an opposite sign.

In the case 3) when $E^\uparrow \gg T_{c0}$ and $E^\downarrow \ll T_{c0}$, the electrons with spin up have a strong energy band shift compared to the superconducting energy spectrum and the electrons with spin down a very small one. The critical temperature difference becomes $\Delta T/T_c^0 = 31E^\downarrow t^4 \zeta(5)/(64\pi^4 T_{c0}^4 E^\uparrow)$. Again the $\pi-$phase appears if $E^\uparrow$ and $E^\downarrow$ have an opposite sign. Here, we note that ΔT depends linearly on $E^\downarrow$. As a consequence, when $E^\downarrow$ goes to zero (superconductor and electrons down ferromagnet energy band coincides) then $T_c^0 = T_c^\pi$ in our approximation and to determine the type of the ground state it is needed to calculate ΔT at higher order over t approximation.

As a conclusion, the $\pi-$phase does not exist if the energy band edges for both spin orientation of the ferromagnet are higher or lower than that of superconductor one. Consequently, the energy shift between the ferromagnet electron band and the superconductor electron band strongly influences the $\pi-$phase existence.

In real compounds, the results depends on the details of the exact form of the Fermi surfaces of superconductor and ferromagnet. Hence, the anisotropy may have an effect on the $0 - \pi$ phase transition.

To illustrate the anisotropic case, we choose elliptic Fermi surface of F layer. The majority and minority energy spectra $\xi^\uparrow(\theta)$ and $\xi^\downarrow(\theta)$ depend on the polar angle θ in the (k_x, k_y) plane (see figure 2).

In the case of strong energy band splitting between ferromagnet and superconductor electron bands, the spectrum of majority (minority) ferromagnet electrons can be written as $\xi^{\uparrow(\downarrow)}(\theta) = \xi_s + E^{\uparrow(\downarrow)}(\theta)$ where ξ_s is the superconducting spectrum considered as isotropic one. In spite of the dependence on θ, the situation depicted in the figures 2 a) and 2 b)
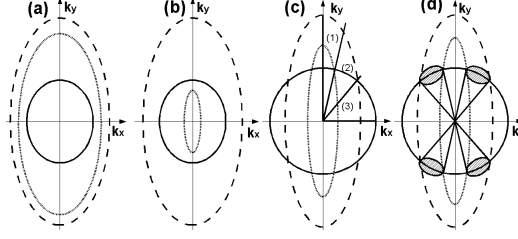
Fig. 2: 2-D Fermi surfaces for superconductor ξ_s (solid line) and for majority $\xi_\uparrow$ and minority $\xi_\downarrow$ bands of ferromagnet (dashed and dotted lines correspondingly). In (a) is depicted the situation where $\xi_s < \xi_\downarrow < \xi_\uparrow$. In (b) is depicted the situation where $\xi_\downarrow < \xi_s < \xi_\uparrow$. In (c) are represented the different areas where the integration are done. In area (1) $\xi_s < \xi_\uparrow < \xi_\downarrow$, in area (2) $\xi_\uparrow < \xi_s < \xi_\downarrow$ and in area (3) $\xi_\uparrow < \xi_\downarrow < \xi_s$. (d) represents the sign of $\ln\left(T_c^0/T_c^\pi\right)$ in the different areas. In the shaded areas, the integral is negative and in the other one, the integral is positive. In the frontier, the integral equals zero.

are similar to the isotropic situation and we can estimate the sign of ΔT without doing the integration over θ. Thereby, the conclusions are the same as in the isotropic case.

From (8), we deduced that $\Delta T > 0$ and the S/F/S trilayer is in the $0-$phase if $E^\uparrow(\theta)$ and $E^\downarrow(\theta)$ have both the same sign for all values of θ e.g. $E^\uparrow(\theta) > 0$ and $E^\downarrow(\theta) > 0$ which corresponding sketch of Fermi surfaces is presented on the figure 2a). Thus, $\Delta T < 0$ and the S/F/S trilayer is in the $\pi-$phase if $E^\uparrow(\theta)$ and $E^\downarrow(\theta)$ have opposite sign for all values of θ e.g. $E^\uparrow(\theta) > 0$ and $E^\downarrow(\theta) < 0$ which corresponding sketch of Fermi surfaces is presented on the figure 2b). Consequently, the anisotropy of electrons band do not influence the $0-\pi$ transition phase when F layers and S layers Fermi surfaces do not intersect.

Let us consider now the case when the F layers and S layers Fermi surfaces intersect (see figure 2 c)). In this case, the intersections delimit the regions where ΔT is positive or negative. In order to estimate the resulting sign of ΔT without integrate over θ, we divide the Fermi surface in three regions. And then, according to the total surface of "positive" and "negative" region, one may conclude which state is realized.

In the regions (1) and (3), both $E^\uparrow(\theta)$ and $E^\downarrow(\theta)$ have the same sign (positive in (1) and negative in (3)). Consequently, ΔT is positive and the S/F/S junctions exhibit a $0-$phase behavior in these regions. In the region (2), $E^\uparrow(\theta)$ and $E^\downarrow(\theta)$ have opposite sign ($E^\uparrow(\theta) > 0$ and $E^\downarrow(\theta) < 0$) so, ΔT is negative and the S/F/S junctions exhibit a $\pi-$phase behavior in these regions.

The sign of the contributions of the each region to ΔT is depicted in the figure 2 (d). If the overall size of the regions where $\pi-$phase is realized is greater than the overall size of the region where the $0-$phase exists, we can conclude that the phase difference between the two superconducting layers is π. In the contrary case, the phase difference between the two superconducting layers is 0. These results implies that the anisotropy of the Fermi surfaces with intersection and energy band shift has an important effect on the $0-\pi$ phase transition.

We may generalize the S/F/S hybrid system by considering an arbitrary number of F layers between the two S layers. In [29], the authors found that the $0-\pi$ phase transition of superconductor-antiferromagnet-superconductor (S-AF-S) junctions manifests a dependence on the number of magnetic atomic layer. The AF interlayer is composed by an even or odd number of monoatomic F layer where each F adjacent layer have an opposite magnetization. At low temperatures the junction S-AF-S is either a 0 or π junction depending on wether the AF interlayer consists of an even or odd number of atomic layers. In this paper, we show that in fact the $0-\pi$ phase transition depends only on the number of ferromagnetic layers between the two S layers but not on the relative orientation of the magnetization between adjacent F layers. We generalize our model by adding $N-2$ F layers between the two S

layers with $n = 0$ and $n = N$. For simplicity, we consider that the ferromagnet spectrum can be written as $\xi_\uparrow = E^\uparrow$ and $\xi_\downarrow = E^\downarrow$ where $E^\uparrow$ and $E^\downarrow$ have opposite sign and $E^{\uparrow(\downarrow)} \gg T_{c0}$. Thus in the limit $t \ll E^{\uparrow(\downarrow)}$ we can express the normal Green function between the layer 0 and the Nth layer like :

$$G^\omega_{0\uparrow\uparrow}(0, N) = \frac{t}{(i\omega - \xi_s)^2} \prod_{n=1}^{N-1} \frac{t}{E^\uparrow_n}.$$

The critical temperature difference following the formular similar to (7) is :

$$\frac{\Delta T}{T_c^0} = \frac{7 t^2 \zeta(3)}{8 \pi^2 T_{c0}^2} \left\{ \prod_{n=1}^{N-1} \frac{t^2}{E^\uparrow_n E^\downarrow_n} \right\}. \tag{9}$$

As it follows from (9) the insertion of each supplementary F layers leads to additional phase shift of π. As a consequence, the resulting phase difference (0 or π) is determined by the number of ferromagnetic layers between the superconductors. If the number of ferromagnetic layers is even the total phase difference φ_t induced by the ferromagnetic layers is $\varphi_t = 2n\pi$ that correspond to a $0-$phase shift. For the odd numbers of ferromagnetic layers the total phase difference is $\varphi_t = (2n+1)\pi$ that means the $\pi-$phase shift. Hence, the magnetization of adjacent ferromagnetic spacers have no influence on the fact that the system is in 0 or -phase in contrast with the result in [29].

4. Spin-switch effect in F/S/F system - In this section, we study the possible inversion of the SSE in a superconductor layer sandwiched by two ferromagnetic adjacent layers in the F/S/F structure (see figure 1b)). We label $n = 0, 2$ so $\xi_{\sigma,0}$ and $\xi_{\sigma,2}$ are the electron spectra for the F layers and $n = 1$ so $\xi_{s,1} = \xi_s$ for the S layer. The BCS Hamiltonian H_{BCS} and the kinetic energy Hamiltonian H_0 are described by (3). In [24], the authors observed the inversion of the SSE (they observed that the critical temperature in the parallel state is higher than in the antiparallel one, $T_{cP} > T_{cAP}$) in $[Co/Pt]/Nb/[Co/Pt]$ structure and proposed an explanation for the inversion of the SSE. In the parallel (P) state the spin-polarized carriers can migrate from one F layer across the intermediate S layer to the other F layer whereas in the antiparallel (AP) state this effect is reduced and the spin polarized carriers is reflected back into the S layer. This means that the transparency of the S-F interfaces depends on the electron spin orientation. In our model, that implies that the transfer energy between two layers may depend on the electron spin orientation so in (3), instead of t one, we introduce two different energy transfer $t_\uparrow$ and $t_\downarrow$ with $t_\uparrow \neq t_\downarrow$. Near T_c, in the isotropic case, the critical temperature equation is [28] :

$$\ln\left(\frac{T_{cP}}{T_{cAP}}\right) = 2T_{cP} \sum_{\omega>0} \int \mathrm{Re}\left(\widetilde{F}_{\downarrow\uparrow,P} - \widetilde{F}_{\downarrow\uparrow,AP}\right) d\xi_s, \tag{10}$$

where $T_{cP(AP)}$ is the superconductor critical temperature in the P (AP) case. Using the Green function formalism and the equations (4) modified with the new tunneling Hamiltonian $H_t^{P(AP)}$, we calculate the anomalous Green function in the S layer in the P state $F^+_{\downarrow\uparrow,P}(1, 1)$ and in the AP state $F^+_{\downarrow\uparrow,AP}(1, 1)$. Expanding this function in power of $t_\uparrow$ and $t_\downarrow$, and keeping the terms proportional to t^4, we obtain the difference of the anomalous Green function $F^+_{\downarrow\uparrow,P} - F^+_{\downarrow\uparrow,AP}$:

$$\widetilde{F}_{\downarrow\uparrow,P} - \widetilde{F}_{\downarrow\uparrow,AP} = \frac{1}{\omega^2+\xi^2}\left[\frac{2}{(i\omega+\xi)^2}\left[\frac{t_\uparrow^2}{i\omega+\xi_\uparrow} - \frac{t_\downarrow^2}{i\omega+\xi_\downarrow}\right]^2\right]$$
$$-\frac{1}{(\omega^2+\xi^2)}\left[\frac{t_\uparrow^4}{(\omega^2+\xi_\uparrow^2)} + \frac{t_\downarrow^4}{(\omega^2+\xi_\downarrow^2)} + \frac{2t_\uparrow^2 t_\downarrow^2}{(\omega^2+\xi^2)(i\omega-\xi_\uparrow)(i\omega+\xi_\downarrow)}\right].$$

We choose for simplicity, the energy spectra for the P case like $\xi_\uparrow \equiv \xi_{\uparrow,0} = \xi_{\uparrow,2}$ and $\xi_\downarrow \equiv \xi_{\downarrow,0} = \xi_{\downarrow,2}$, and for the AP case, $\xi_\uparrow \equiv \xi_{\uparrow,0} = \xi_{\downarrow,2}$ and $\xi_\downarrow \equiv \xi_{\downarrow,0} = \xi_{\uparrow,2}$. The sign
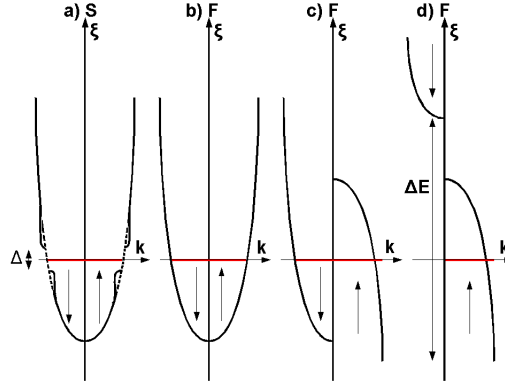
Fig. 3: (a) Spectrum of a superconducting metal (b) Spectrum of a normal metal where $\xi_\uparrow = \xi_\downarrow = \xi_s$. (c) Spectrum of a strong ferromagnet with reversed spectrum where $\xi_\uparrow = -\xi_s$ and $\xi_\downarrow = \xi_s$. (d) Spectrum of a strong ferromagnet with a reversed spectrum where $\xi_\uparrow = -\xi_s$ and $\xi_\downarrow = \Delta E \gg k_B T_c$.

of the right hand part in (10) determines whether we deal with normal or inverse SSE. In particular, if $\ln(T_{cP}/T_{cAP})$ is positive then $T_{cP} > T_{cAP}$ and so the SSE is reversed.

To verify the hypothesis of [24] , we consider first the spectra $\xi_\uparrow = \xi_\downarrow = \xi_s$, see figure 3 b) and we find :

$$\frac{\Delta T}{T_{cP}} = -\frac{31}{64}\frac{\zeta(5)}{\pi^4 T_{cp}^4}\left(t_\downarrow^2 - t_\uparrow^2\right)^2 \tag{11}$$

where we have introduced for this section $\Delta T = T_{cP} - T_{cAP}$ and $\zeta(5) = 1.03$. We see that the right hand side of equation (11) is always negative. It is the normal SSE. We choose another spectra $\xi_\uparrow = \xi_s$ and $\xi_\downarrow = \Delta E$ with $\Delta E \gg T_c$, then the critical temperature difference becomes :

$$\frac{\Delta T}{T_{cP}} = -\frac{1}{64}\frac{\left[31\zeta(5)t_\uparrow^4 \Delta E^2 + 112 t_\downarrow^4 \zeta(3)\pi^2 T_{cP}^2\right]}{\Delta E^2 \pi^4 T_{cp}^4}. \tag{12}$$

The right hand side of (12) is always negative so $T_{cP} < T_{cAP}$. Consequently, the superconductor critical temperature in the P case is always lower than in the AP case, $T_{cP} < T_{cAP}$. It is the normal SSE.

Thus, the hypothesis on the difference between $t_\uparrow$ and $t_\downarrow$ cannot explain the inversion of the SSE. Nevertheless, in strong ferromagnetic, the inversion of the electron spectrum provides another possibility to explain this unusual behavior.

Indeed, in the case of strong ferromagnet, the band splitting can be so important that one of the electron band (here the spin up band) becomes a hole-like (see figure 3 c)). Here, the exchange field triggers the hole-like energy band for spin up electrons but do not appear explicitly in the calculation. That's allows us to emphasize the important influence of inverse spectra on T_c. In the very special case where the electron spectra can be written as $\xi_\uparrow = -\xi_s$ and $\xi_\downarrow = \xi_s$, we find :

$$\frac{\Delta T}{T_{cP}} = \frac{31}{128}\frac{\zeta(5)}{\pi^4 T_{cp}^4}\left(3t_\uparrow^4 - 2t_\downarrow^4 - 4t_\downarrow^2 t_\uparrow^2\right). \tag{13}$$

If we put $t_{\uparrow(\downarrow)} = t_0 \pm \Delta t$ then ΔT is positive $(T_{cP} > T_{cAP})$ and the spin-switch effect is reversed if $\Delta t \gtrsim 0.1 t_0$ (see figure 4(a)). We notice that the spin-switch effect is reversed if $t_\downarrow = 0$ and normal if $t_\uparrow = t_\downarrow$. Hence, we verify that the condition $t_\uparrow \neq t_\downarrow$ cannot explain alone the inversion of SSE and have to be associated with the inversion of majority electron energy band.

The minority electron band can be shifted considerably compared to the superconductor spectrum (see figure 3 d)). In this case, the spectra are $\xi_\uparrow = -\xi_s$ and $\xi_\downarrow = \Delta E \gg T_c$. This
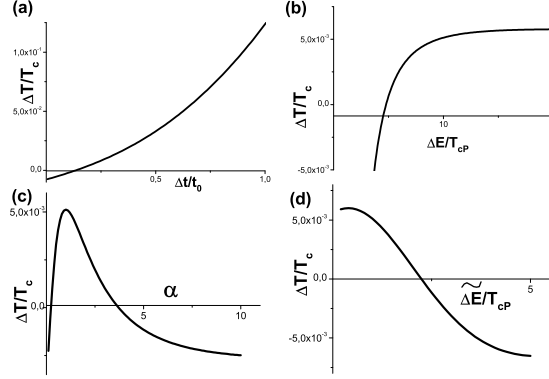
Fig. 4: (a) $\Delta T/T_c$ as a function of $\Delta t/t_0$ is presented in the units of $(t_0/T_c)^4$ in the situation $\xi_\uparrow = -\xi_s$ and $\xi_\downarrow = \xi_s$. (b) $\Delta T/T_c$ as a function of $\Delta E/T_c$ presented in the units of $(t/T_c)^4$ with $t_\uparrow = t_\downarrow = t$, in the situation $\xi_\uparrow = -\xi_s$ and $\xi_\downarrow = \Delta E \gg T_c$. (c) $\Delta T/T_c$ as a function of α presented in the units of $(t/T_c)^4$ with $t_\uparrow = t_\downarrow = t$, $\Delta E = 10T_c$ and $\widetilde{\Delta E} = T_c$ in the situation $\xi_\uparrow = -\alpha.\xi_s + \widetilde{\Delta E}$ and $\xi_\downarrow = \Delta E \gg T_c$. (d) $\Delta T/T_c$ as a function of $\widetilde{\Delta E}/T_c$ presented in the units of $(t/T_c)^4$ with $\Delta E = 10T_c$, $t_\uparrow = t_\downarrow = t$ and $\alpha = 1$ in the situation $\xi_\uparrow = -\alpha.\xi_s + \widetilde{\Delta E}$ and $\xi_\downarrow = \Delta E \gg T_c$.

situation gives :

$$\frac{\Delta T}{T_{cP}} = \frac{93}{128}\frac{\zeta(5)}{\pi^4 T_{cp}^4}t_\uparrow^4 - \frac{7\zeta(3)}{4(\Delta E)^2\pi^2 T_{cP}^2}t_\downarrow^4 \tag{14}$$

Therefore ΔT is positive ($T_{cP} > T_{cAP}$) for high ΔE and any relation between $t_\uparrow$, $t_\downarrow$ and the opposite situation realizes if ΔE is small (see figure 4(b)). In the situation of high ΔE, the inversion of SSE is related to the inversion of spectrum of majority electrons. We see that strong energy shifts ΔE between F and S layers favored the inversion of the SSE.

We perform numerical calculation of ΔT in the case of spectra like $\xi_\uparrow = -\alpha.\xi_s + \widetilde{\Delta E}$ and $\xi_\downarrow = \Delta E \gg T_c$ where α is a positive parameter which represents the difference of effective mass between majority and minority electron and $\widetilde{\Delta E}$ is energy shift between electrons up and the superconductor spectrum. For simplicity, we consider $\widetilde{\Delta E} \simeq T_c$ and $t_\uparrow = t_\downarrow = t$. For important or small difference of effective mass, there is no inversion of SSE (see figure 4(c)). The inverse SSE is favored when $\alpha \approx 1$. Hence, the inversion of the SSE is more efficient if the effective mass are close.

The dependence on $\widetilde{\Delta E}$ (see figure 4(d)) shows that the inverse SSE disappears if $\widetilde{\Delta E} \gtrsim 2T_c$. Thus, if the energy shift on the reversed electron energy band is too important then the inverse SSE disappears. This condition is quite restrictive for the appearance of the inversion of the SSE.

5. Conclusions- We have demonstrated an important influence of the spectrum anisotropy of F layers and energy shift between F and S energy spectra on the F/S hetero-structures properties.

For the S/F/S sandwiches, we have shown that the $\pi-$phase cannot appear if the energy shift between S and F spectra is too important. Moreover, on the example of elliptic Fermi surfaces, we show that the anisotropy of F layer spectra may provide rather restrictive conditions of existence of the $\pi-$phase. We have also considered a more general S/F/S structure by including several F layers between the two S layers. The $0-\pi$ phase transition is influenced by the even or odd number of F layer independently of the relative magnetization between adjacent F layer.

For the F/S/F trilayers, we propose a possible explanation of the previously observed

inverse SSE. In strong ferromagnet, the high energy band splitting may imply an inversion of one of the electron energy band. This type of electron spectrum in F layer could explain the anomalous SSE. We also study the influence of the effective mass difference and the energy shift on the inverse spectra.

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